Welcome to STN International! Enter x:x

LOGINID:ssptayvv1621

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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                        Welcome to STN International
NEWS
                   Web Page for STN Seminar Schedule - N. America
NEWS 2 OCT 02 CA/Caplus enhanced with pre-1907 records from Chemisches
                   Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN

NEWS 8 DEC 14 BEILSTEIN pricing structure to change

NEWS 9 DEC 17 USPATOLD added to additional database clusters

NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN

NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
                   MEDLINE segment
NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14 DEC 17 CA/Caplus enhanced with new custom IPC display formats
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
                   from USPATOLD
NEWS 16 JAN 02
                   STN pricing information for 2008 now available
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
                   prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
                   custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
                   of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                   U.S. National Patent Classification
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NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

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NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
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Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 15:16:35 ON 19 MAR 2008

=> file req

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:17:21 ON 19 MAR 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 18 MAR 2008 HIGHEST RN 1008796-87-9 DICTIONARY FILE UPDATES: 18 MAR 2008 HIGHEST RN 1008796-87-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10584221-limited-halogeneation.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 11

MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 2.30 2.51

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 15:20:16 ON 19 MAR 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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FILE CONTENT: 1840 - 15 Mar 2008 VOL 148 ISS 12

New CAS Information Use Policies, enter HELP USAGETERMS for details.

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 11

SAMPLE SEARCH INITIATED 15:20:22 FILE 'CASREACT'

SCREENING COMPLETE - 517 REACTIONS TO VERIFY FROM 35 DOCUMENTS

100.0% DONE 517 VERIFIED 0 HIT RXNS 0 DOCS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 8977 TO 11703 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s 11 full

FULL SEARCH INITIATED 15:20:27 FILE 'CASREACT'

SCREENING COMPLETE - 8713 REACTIONS TO VERIFY FROM 711 DOCUMENTS

100.0% DONE 8713 VERIFIED 20 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.04

L3 1 SEA SSS FUL L1 (20 REACTIONS)

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 117.96 120.47

FILE 'CAPLUS' ENTERED AT 15:20:40 ON 19 MAR 2008
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FILE COVERS 1907 - 19 Mar 2008 VOL 148 ISS 12 FILE LAST UPDATED: 18 Mar 2008 (20080318/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> d 13 ibib abs hit str 1-YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

'STR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

```
ABS ---- GI and AB
ALL ----- BIB, AB, IND, RE, Single-step Reactions
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data
CAN ----- List of CA abstract numbers without answer numbers
CBIB ---- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IND ----- Indexing data
IPC ----- International Patent Classifications
ISTD ----- STD, indented with text labels
OBIB ---- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
MAX ----- Same as ALL
PATS ----- PI, SO
SCAN ----- TI and FCRD (random display, no answer number. SCAN
            must be entered on the same line as DISPLAY, e.g.,
            D SCAN.)
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for
            all single-step reactions)
STD ---- BIB, IPC, and NCL
CRD ----- Compact Display of All Hit Reactions
CRDREF ---- Compact Reaction Display and SO, PY for Reference
FHIT ---- Reaction Map, Diagram, and Summary for first
            hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ----- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
            CA reference information (SO, PY). (Default)
FPATH ----- PATH, plus Reaction Summary for the "long path"
FSPATH ---- SPATH, plus Reaction Summary for the "short path"
HIT ----- Reaction Map, Reaction Diagram, and Reaction
            Summary for all hit reactions and fields containing
            hit terms
```

OCC ----- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications. PATH ---- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions) RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions) RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions) RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions) SPATH ----- Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d 13 ibib abs hitstr 1-YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

```
ABS ---- GI and AB
ALL ----- BIB, AB, IND, RE, Single-step Reactions
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IND ----- Indexing data
IPC ----- International Patent Classifications
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
MAX ----- Same as ALL
PATS ----- PI, SO
SCAN ----- TI and FCRD (random display, no answer number. SCAN
            must be entered on the same line as DISPLAY, e.g.,
```

D SCAN.) SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions) STD ----- BIB, IPC, and NCL CRD ----- Compact Display of All Hit Reactions CRDREF ---- Compact Reaction Display and SO, PY for Reference FHIT ---- Reaction Map, Diagram, and Summary for first hit reaction FHITCBIB --- FHIT, AN plus CBIB FCRD ----- First hit in Compact Reaction Display (CRD) format FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default) FPATH ----- PATH, plus Reaction Summary for the "long path" FSPATH ---- SPATH, plus Reaction Summary for the "short path" HIT ---- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms OCC ----- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications. PATH ----- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions) RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions) RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions) RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions) SPATH ---- Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

within another hit reaction which is displayed

ENTER DISPLAY FORMAT (FCRDREF):end

=> d 13 ibib abs
YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 135:344284 CASREACT

TITLE: Process for the preparation of 2-halobenzoic acids by

 $\verb"palladium-catalyzed regioselective halogenation" of$

benzoic acids

INVENTOR(S): Kodama, Hiroki; Katsuhira, Takeshi; Nishida, Tateki;

Hino, Tomokazu; Tsubata, Kenji

PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

Ρ.	PATENT NO.					ND	DATE			A.	PPLI	CATI	и ис	0.	DATE						
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OTHER SOURCE(S): MARPAT 135:344284

GI

AB A process for the preparation of 2-halobenzoic acids of the general formula [I; A is OH, OM (wherein M is an alkali metal), or NR6R7 (wherein R6 and R7 are each H, C1-6 alkyl, optionally substituted Ph, or the like); R is H, C1-6 alkyl, C1-6 alkylcarbonyl, carboxyl, C1-12 alkoxycarbonyl, optionally substituted phenylcarbonyl, or the like; n is 0 to 4; and X is Cl, Br, or iodo, or alternatively nR's may be present on benzene-constituting carbon atoms adjacent to each other and form a C3-4 alkylene or C3-4 alkenylene-fused ring.] is characterized by reacting a benzoic acid of the general formula I (X = H; A, R, n = same as above) with a halogenating agent in the presence of a Pd catalyst. This process provides regioselective halogenation under mild conditions. Thus, 0.3 g o-toluic acid, 0.5 g N-iodosuccinimide, and 11 mL DMF were added to 50 mg Pd(OAc)2

in a 50 mL glass reaction vessel and stirred at 100° for 6 h to give 92% 2-iodo-6-methylbenzoic acid with 100% regioselectivity.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 1.44 127.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE

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-0.75

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STRUCTURE FILE UPDATES: 18 MAR 2008 HIGHEST RN 1008796-87-9 DICTIONARY FILE UPDATES: 18 MAR 2008 HIGHEST RN 1008796-87-9

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10584221-product.str

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 15:24:02 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 11999 TO ITERATE

16.7% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

36 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 233416 TO 246544 PROJECTED ANSWERS: 3438 TO 5200

T.5 36 SEA SSS SAM L4

=> s 14 full

FULL SEARCH INITIATED 15:24:06 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 241591 TO ITERATE

100.0% PROCESSED 241591 ITERATIONS 3471 ANSWERS

SEARCH TIME: 00.00.04

L6 3471 SEA SSS FUL L4

Uploading C:\Program Files\Stnexp\Queries\10584221-start-mat.str

STRUCTURE UPLOADED L7

=> s 17 full

FULL SEARCH INITIATED 15:25:30 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 338183 TO ITERATE

100.0% PROCESSED 338183 ITERATIONS 9591 ANSWERS

SEARCH TIME: 00.00.11

9591 SEA SSS FUL L7

=> file caplus

SINCE FILE TOTAL ENTRY SESSION 357.64 485.13 COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

0.00 -0.75 CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 19 Mar 2008 VOL 148 ISS 12 FILE LAST UPDATED: 18 Mar 2008 (20080318/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 16 and 18

155 L6

1702 L8

L9 52 L6 AND L8

=> s 19 and catalyst

794610 CATALYST

L10 2 L9 AND CATALYST

=> s 19 and palladium

175682 PALLADIUM

L11 2 L9 AND PALLADIUM

=> s 110 or 111

L12 2 L10 OR L11

=> d 112 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:612248 CAPLUS

DOCUMENT NUMBER: 143:133190

TITLE: Process for the preparation of 2-halogenobenzamide

derivatives

INVENTOR(S): Abe, Noboru; Kodama, Hiroki; Yoshiura, Akihiko

PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P.	ATENT	NO.	KIN	KIND DATE					LICAT	DATE							
W(√O 2005063703				A1	_	2005	0714						20041222			
	W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	ΒA,	BB	, BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	, EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	, KE,	KG,	KP,	KR,	KΖ,	LC,	LK,
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK	, MN,	MW,	MX,	MZ,	NA,	NI,	NO,
		NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC	, SD,	SE,	SG,	SK,	SL,	SY,	ТJ,
		TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	, VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MΖ,	NA,	SD	, SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	AT,	, BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	, IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	, CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,
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										WO 2	2004-	JP19	234		W 2	0041	222
OTHER 9	SOURCE		MAR.	PAT	143.	1331	9 N										

OTHER SOURCE(S): MARPAT 143:133190

GΙ

Ι

AB A process for the preparation of title compds. of formula I [Y = Cl, Br or iodo; Rl-R4, R6 = independently H or alkyl; R5 = alkyl; m = 2; n = 1 or 2; Yl-Y4 = independently H, halo, cyano, nitro, alkyl, etc.] comprising reacting a compound I (Y = H, m = 0 or 1, the others are defined as above) with a halogenating agent in the presence of a palladium catalyst and then reacting with an oxidizing agent is disclosed. For example, II was given in a multi-step synthesis starting from phthalic acid anhydride. The title compound is useful as a raw material or active ingredient for medicines and agricultural chems. (no data).

IT 371771-01-6P 371771-07-2P 858658-99-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-halogenobenzamide derivs. by Pd-catalyzed halogenation and oxidation of correspond benzamides)

RN 371771-01-6 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CFINDEX NAME)

RN 371771-07-2 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 858658-99-8 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-N'-(2,3,4-trichlorophenyl)- (9CI) (CA INDEX NAME)

IT 272451-63-5P 272451-65-7P 474558-18-4P

858658-98-7P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-halogenobenzamide derivs. by Pd-catalyzed halogenation and oxidation of correspond benzamides)

RN 272451-63-5 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylsulfonyl)ethyl]-3-iodo-N1-[2-methyl-4-(pentafluoroethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 272451-65-7 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylsulfonyl)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 474558-18-4 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylsulfonyl)ethyl]-3-iodo-N1-(2,3,4-trichlorophenyl)- (CA INDEX NAME)

RN 858658-98-7 CAPLUS

CN Benzamide, N-[1,1-dimethyl-2-(methylsulfonyl)ethyl]-2-iodo-6-methyl- (CA INDEX NAME)

IT 858659-00-4 858659-01-5

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of 2-halogenobenzamide derivs. by Pd-catalyzed halogenation and oxidation of correspond benzamides)

RN 858659-00-4 CAPLUS

CN Benzamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-2-methyl- (CA INDEX NAME)

RN 858659-01-5 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-N'-[2-

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:816609 CAPLUS

DOCUMENT NUMBER: 135:344284

TITLE: Process for the preparation of 2-halobenzoic acids by

palladium-catalyzed regioselective

halogenation of benzoic acids

INVENTOR(S): Kodama, Hiroki; Katsuhira, Takeshi; Nishida, Tateki;

Hino, Tomokazu; Tsubata, Kenji

PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	TENT	NO.			KIN	D	DATE		APPLICATION NO.						DATE			
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OTHER SOURCE(S): CASREACT 135:344284; MARPAT 135:344284

AΒ A process for the preparation of 2-halobenzoic acids of the general formula [I; A is OH, OM (wherein M is an alkali metal), or NR6R7 (wherein R6 and R7 are each H, C1-6 alkyl, optionally substituted Ph, or the like); R is H, C1-6 alkyl, C1-6 alkylcarbonyl, carboxyl, C1-12 alkoxycarbonyl, optionally substituted phenylcarbonyl, or the like; n is 0 to 4; and X is Cl, Br, or iodo, or alternatively nR's may be present on benzene-constituting carbon atoms adjacent to each other and form a C3-4 alkylene or C3-4alkenylene-fused ring.] is characterized by reacting a benzoic acid of the general formula I (X = H; A, R, n = same as above) with a halogenating agent in the presence of a Pd catalyst. This process provides regioselective halogenation under mild conditions. Thus, 0.3 g o-toluic acid, 0.5 g N-iodosuccinimide, and 11 mL DMF were added to 50 mg Pd(OAc)2 in a 50 mL glass reaction vessel and stirred at 100° for 6 h to give 92% 2-iodo-6-methylbenzoic acid with 100% regioselectivity. 317812-34-3, 2-(((1,1-Dimethyl-2-methylsulfinylethyl)amino)carbonyΙT 1) - N - (6 - (1, 1, 1, 3, 3, 3 - hexafluoropropan - 2 - yloxy) - 2 - methylpyridin - 3 - (6 - (1, 1, 1, 3, 3, 3, 3 - hexafluoropropan))yl)benzamide 371771-01-6 371771-03-8 371771-05-0 371771-07-2 371771-08-3, 2-(((1,1-Dimethyl-2-methylsulfinylethyl)amino)carbonyl)benzoic acid methyl ester 371771-18-5, N-(1,1-Dimethyl-2-methylthioethyl)-2nitrobenzamide 371771-20-9 371771-22-1 371771-24-3 371771-26-5 371771-28-7 371771-30-1 371771-32-3 371771-34-5, 2-(4-Chloro-2-methylphenoxy)-N-(1,1-dimethyl-2-methylthioethyl)benzamide 371771-36-7, 2-(3-Chloro-5-trifluoromethylpyridin-2-yloxy)-N-(1,1dimethyl-2-methylthioethyl) benzamide 371771-38-9, 2-(4,6-Dimethoxypyrimidin-2-yloxy)-N-(1,1-dimethyl-2methylthioethyl) benzamide 371771-40-3, 2-(4-Trifluoromethylphenyl)-N-(1,1-dimethyl-2-methylthioethyl)benzamide 371771-42-5, 2-(4-Trifluoromethylphenyl)-N-(1,1-dimethyl-2-matmethylsulfinylethyl) benzamide 371771-51-6, 2-(((1,1-Dimethyl-2methylsulfinylethyl)amino)carbonyl)benzoic acid n-butyl ester RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of 2-halobenzoic acids by regioselective halogenation of benzoic acids in presence of palladium compound) 317812-34-3 CAPLUS RN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-N'-[2-CN

methyl-6-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-3-pyridinyl]- (9CI) (CA INDEX NAME)

RN 371771-01-6 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 371771-03-8 CAPLUS

CN 2,3-Naphthalenedicarboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 371771-05-0 CAPLUS

CN 1,2-Benzenedicarboxamide, 4-chloro-N2-[1,1-dimethyl-2-(methylthio)ethyl]- N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-07-2 CAPLUS

CN 1,2-Benzenedicarboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 371771-08-3 CAPLUS

CN Benzoic acid, 2-[[[1,1-dimethyl-2-(methylsulfinyl)ethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

RN 371771-18-5 CAPLUS

CN Benzamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-2-nitro- (CA INDEX NAME)

RN 371771-20-9 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-4-fluoro-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-22-1 CAPLUS

CN 1,2-Benzenedicarboxamide, 4-chloro-N1-[1,1-dimethyl-2-(methylthio)ethyl]-N2-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-24-3 CAPLUS

CN 1,2-Benzenedicarboxamide, 4-bromo-N1-[1,1-dimethyl-2-(methylthio)ethyl]-N2[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA
INDEX NAME)

RN 371771-26-5 CAPLUS

CN 1,2-Benzenedicarboxamide, N1-[1,1-dimethyl-2-(methylthio)ethyl]-4-methyl-N2-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-28-7 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-4-methoxy-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-30-1 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

RN 371771-32-3 CAPLUS

CN 1,8-Naphthalenedicarboxamide, N-[1-methyl-2-(methylthio)ethyl]-N'-[2-methyl-4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 371771-34-5 CAPLUS

CN Benzamide, 2-(4-chloro-2-methylphenoxy)-N-[1,1-dimethyl-2-(methylthio)ethyl]- (CA INDEX NAME)

RN 371771-36-7 CAPLUS

CN Benzamide, 2-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]-N-[1,1-dimethyl-2-(methylthio)ethyl]- (CA INDEX NAME)

RN 371771-38-9 CAPLUS

CN Benzamide, 2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-N-[1,1-dimethyl-2-(methylthio)ethyl]- (CA INDEX NAME)

RN 371771-40-3 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-4'-(trifluoromethyl)- (CA INDEX NAME)

RN 371771-42-5 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-4'-(trifluoromethyl)- (CA INDEX NAME)

RN 371771-51-6 CAPLUS

CN Benzoic acid, 2-[[[1,1-dimethyl-2-(methylsulfinyl)ethyl]amino]carbonyl]-, butyl ester (CA INDEX NAME)

ΙT 272451-61-3P 272451-69-1P 317812-12-7P, 2-(((1,1-Dimethyl-2-methylsulfinylethyl)amino)carbonyl)-N-(6-(1,1,1,3,3,3-1))hexafluoropropan-2-yloxy)-2-methylpyridin-3-yl)-3-iodobenzamide 371771-04-9P 371771-06-1P 371771-09-4P, 3-Iodo-2-(((1,1-dimethyl-2-methylsulfinylethyl)amino)carbonyl)benzoic acid methyl ester 371771-19-6P, N-(1,1-Dimethyl-2-methylthioethyl)-2iodo-6-nitrobenzamide 371771-21-0P 371771-23-2P 371771-25-4P 371771-27-6P 371771-29-8P 371771-31-2P 371771-33-4P 371771-35-6P, 2-(4-Chloro-2-methylphenoxy)-N-(1,1-dimethyl-2-methylthioethyl)-6iodobenzamide 371771-37-8P, 2-(3-Chloro-5-trifluoromethylpyridin-2-yloxy)-N-(1,1-dimethyl-2-methylthioethyl)-6-iodobenzamide 371771-39-0P, 2-(4,6-Dimethoxypyrimidin-2-yloxy)-N-(1,1-dimethyl-2-yloxy)methylthioethyl)-6-iodobenzamide 371771-41-4P, 2-(4-Trifluoromethylphenyl)-6-iodo-N-(1,1-dimethyl-2methylthioethyl) benzamide 371771-43-6P, 2-(4-Trifluoromethylphenyl)-6-iodo-N-(1,1-dimethyl-2methylsulfinylethyl)benzamide 371771-52-7P, 2-(((1,1-Dimethyl-2methylsulfinylethyl)amino)carbonyl)-3-iodobenzoic acid n-butyl ester RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 2-halobenzoic acids by regioselective halogenation of

benzoic acids in presence of palladium compound)

RN 272451-61-3 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 272451-69-1 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 317812-12-7 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-3-iodo-N1-[2-methyl-6-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]-3-pyridinyl]-(CA INDEX NAME)

RN 371771-04-9 CAPLUS

CN 2,3-Naphthalenedicarboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-1-iodo-N'-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 371771-06-1 CAPLUS

CN 1,2-Benzenedicarboxamide, 4-chloro-N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-(CA INDEX NAME)

RN 371771-09-4 CAPLUS

CN Benzoic acid, 2-[[[1,1-dimethyl-2-(methylsulfinyl)ethyl]amino]carbonyl]-3-iodo-, methyl ester (CA INDEX NAME)

RN 371771-19-6 CAPLUS

CN Benzamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-2-iodo-6-nitro- (CA INDEX NAME)

RN 371771-21-0 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-4-fluoro-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-(CA INDEX NAME)

RN 371771-23-2 CAPLUS

CN 1,2-Benzenedicarboxamide, 5-chloro-N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-(CA INDEX NAME)

RN 371771-25-4 CAPLUS

CN 1,2-Benzenedicarboxamide, 5-bromo-N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-(CA INDEX NAME)

RN 371771-27-6 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-5-methyl-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-29-8 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-4-methoxy-N1-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (CA INDEX NAME)

RN 371771-31-2 CAPLUS

CN 1,2-Benzenedicarboxamide, N2-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-N1- [2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-4- (trifluoromethoxy)- (CA INDEX NAME)

RN 371771-33-4 CAPLUS

CN 1,8-Naphthalenedicarboxamide, 2-iodo-N1-[1-methyl-2-(methylthio)ethyl]-N8-[2-methyl-4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)

RN 371771-35-6 CAPLUS

CN Benzamide, 2-(4-chloro-2-methylphenoxy)-N-[1,1-dimethyl-2-(methylthio)ethyl]-6-iodo- (CA INDEX NAME)

RN 371771-37-8 CAPLUS

CN Benzamide, 2-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]oxy]-N-[1,1-dimethyl-2-(methylthio)ethyl]-6-iodo- (CA INDEX NAME)

RN 371771-39-0 CAPLUS

CN Benzamide, 2-[(4,6-dimethoxy-2-pyrimidinyl)oxy]-N-[1,1-dimethyl-2-(methylthio)ethyl]-6-iodo- (CA INDEX NAME)

RN 371771-41-4 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[1,1-dimethyl-2-(methylthio)ethyl]-3-iodo-4'-(trifluoromethyl)- (CA INDEX NAME)

RN 371771-43-6 CAPLUS

CN [1,1'-Biphenyl]-2-carboxamide, N-[1,1-dimethyl-2-(methylsulfinyl)ethyl]-3-iodo-4'-(trifluoromethyl)- (CA INDEX NAME)

RN 371771-52-7 CAPLUS

CN Benzoic acid, 2-[[[1,1-dimethyl-2-(methylsulfinyl)ethyl]amino]carbonyl]-3-iodo-, butyl ester (CA INDEX NAME)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT